New Global Minima for Thomson's Problem of Charges on a Sphere

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Abstract

Using numerical arguments we find that for $N = 306$ a tetrahedral configuration (T_h) and for $N = 542$ a dihedral configuration (D_5) are likely the global energy minimum for Thomson's problem of minimizing the energy of N unit charges on the surface of a unit conducting sphere. These would be the largest N by far, outside of the icosadeltahedral series, for which a global minimum for Thomson's problem is known. We also note that the current theoretical understanding of Thomson's problem does not rule out a symmetric configuration as the global minima for $N = 306$ and 542. We explicitly find that analogues of the tetrahedral and dihedral configurations for N larger than 306 and 542, respectively, are not global minima, thus helping to confirm the theory of Dodgson and Moore (Phys. Rev. B 55, 3816 (1997)) that as N grows dislocation defects can lower the lattice strain of symmetric configurations and concomitantly the energy. As well, making explicit previous work by ourselves and others, for $N < 1000$ we give a full accounting of icosadeltahedral configuration which are not global minima and those which appear to be, and discuss how this listing and our results for the tetahedral and dihedral configurations may be used to refine theoretical understanding of Thomson's problem.

What configuration of N unit charges on the (surface) of a unit conducting sphere minimizes the Coulombic energy $\sum_{i \neq j} 1/r_{ij}$ [1]? Beyond physics this question has utility in assembly of biological [2] and chemical structures [3, 4], to benchmark optimization algorithms, and, as well, in mathematics Smale [5] has noted this question to be a *Hilbert problem* for the Twenty-First Century. For $2 \leq N \leq 100$, the original question asked by J.J. Thomson a century ago, and a bit beyond, there is agreement of all numerical [6, 7, 8, 9, 10] and theoretical [11] methods suggesting that the global minimum configuration has been found. However, for larger N owing to an exponential growth in good local minima [7], finding global minima, general principles or insights for minimization, or even methods or cases to test hypotheses has proven extremely difficult. For $N = 10(h^2 + k^2 + hk) + 2$ highly symmetric icosadeltahedral configurations can be constructed. While it was initially thought that such configurations might be global minima [12], for large N adding defects to the icosadeltahedral lattice lowers the energy [13, 14, 15, 16, 17]. Here we note a tetrahedral configuration for $N = 306$ and a dihedral configuration for $N = 542$ which based on numerical arguments appear to be global minima, the largest such N by far, aside from the icosadeltahedral series, for which a global energy minimum configuration is known. Study of tetrahedral analogues larger than 306 and dihedral analogues larger than 542 help confirm the theory [18] on defects lowering lattice strain and energy. As well, we note that the fact that lattice configurations fail to be global minima for $N > 800$, may help explain why Mo_{154} anions self-assemble into a spherical superstructure with a non-lattice number of subunits [4].

For $N = 78$, as originally suggested by Edmunson [11], the presumed global minimum configuration has tetrahedral (T_h) symmetry (Figure 1a) [7, 8, 9, 10, 11]. We had previously suggested that an analogue of this configuration with 306 charges (Figure 1b, see below for method of construction of this analogue) also might be a global minimum and done limited numerical testing of this idea [12]. Now, here we have extensively checked numerically on over one thousand runs, and have found no configuration of lower energy. (Numerically to look for non-lattice configurations with energies lower than the lattice configuration we used random initial configurations followed by a local steepest descent method. For $N = 306$ we could not find a configuration in one thousand runs with an energy lower than the lattice energy, though for many other N considered in this paper including $N = 1218$ and 4866, and smaller N with icosadeltahedral lattices (see Tables I and II, and Figure 2) configurations

with energies lower than the lattice energy could be found in only fifteen runs.) But one thousand runs is orders of magnitude less than the estimated [7] over 1.5 million local minima for $N = 306$. As well, without an analytic proof we could not be certain the tetrahedral configuration in Figure 1b is the one of minimum energy for $N = 306$. Current theoretical understanding of Thomson's problem [13, 16, 17, 18, 19], to be discussed below, does not exclude the possibility of a symmetric configuration as the global energy minimum for $N = 306$. Of course, our configuration stands open to challenge.

Using a genetic algorithm Morris, Deaven and Ho [9] confirmed previously found [10] presumed global minima for $N \leq 112$ and gave their likely global minima for $N \leq 200$. Fitting the energy of these minima for $N \leq 200$ to the function: $E = N^2/2 \left(1 + aN^{-1/2} + bN^{-3/2}\right)$, (see [9] and refs. therein for an explanation of why this function was used) for $N > 100$ they found particularly deep minima with respect to this function for icosadeltahedral configurations for $N = 122$, 132 192 and for dihedral D_5 configurations for $N = 137$, 182 and 187 and D_2 configuration for N = 146. By our numerical testing as well these dihedral configurations appear to be global minima, though we have no analytic proof and numerically we are orders of magnitude short [7] to even sample a majority of local minima. We next looked at the higher split analogues of these dihedral configurations with $4N - 6$ charges. (See below for the method of construction of such analogues.) The next larger dihedral analogues for $N = 146$, 182 and 187–$N = 578$, 722, and 742 respectively–are found not to be global minima after only a few runs (E.L.A. and A.P.G. data not shown). However, the next larger dihedral (D_5) analogue of $N = 137$–$N = 542$–after over one thousand runs appears possibly to be a global minima. As for the tetrahedral configuration for $N = 306$, we have no analytic proof of this proposition and given the huge number of local minima for an N this large [7] our numerical runs only begin to address the question. Conversely, we easily found that the next analogue of $N = 137$, $N = 2162$, is explicitly not a global energy minimum. See Figure 3 for dihedral configurations for $N = 137$, 542 and 2162.

Euler's theorem asserts that when a (convex) polyhedron is constructed by joining points on a sphere the number of faces (F) plus the number of vertices (V) is equal to the number of edges $(E) + 2$; $F + V = E + 2$. For $N > 12$ this has the result that in addition to the sixfold coordinated points of a planar two-dimensional lattice (hexamers), there must be at least twelve points of fivefold coordination (pentamers). The tetrahedral configurations for $N = 78$ and 306, dihedral configurations for $N = 137$ and 542, and icosadeltahedral

configurations for $N = 10(h^2 + k^2 + hk) + 2$ have exactly twelve pentamers and the rest hexamers (see, e.g., Figure 1a, b, c, e, Figure 2a, b and Figure 3a, b, c). Larger analogues (*split* configurations) of the tetrahedral configuration for $N = 78$ (for $N = $306, 1218, 4886 and for the dihedral configuration for $N = 137$ ($N = 542$, 2162) (Figure 1b, c, e and Figure 3b, c) are made as follows: in addition to the N charges preexisting place one charge at the center of each of the $3N - 6$ edges. (If all the charges were sixfold coordinated hexamers there would be $3N$ edges, six must be subtracted from this to take into account the twelve fivefold coordinated pentamers.) Then relax to the final position by a local gradient method. The resulting configuration has $N + (3N - 6) = 4N - 6$ charges. (See Figure 1b, c, e). Some icosadeltahedral configurations can be made (*split*) as analogues of smaller ones (see e.g. $N = 1242$ in Figure 2b, a larger analogue of $N = 312$ in Figure 2a). A method for making icosadeltahedral configurations *de novo* has been discussed previously [12].

Conversely, to the cases of $N = 78$ and 306, and $N = 137$ and 542 for the larger analogues we have studied ($N = 1218, 4886, 2162$) we find that adding dislocation defects to the lattice produces a configuration with lower energy (Fig. 1$c - f$ and Fig. 3c, d). Similarly, for $N > 792$ icosadeltahedral configurations with dislocation defects, additional fivefold coordinated points and then necessary also sevenfold coordinated points (septamers), have lower energy than symmetric lattice configurations, while for smaller N the symmetric lattice configurations appear to be global minima (see Tables I and II, see Figure 2 for an example), though further numerical testing may show that some such configurations are not global minima.

These numerical results on the N at which tetrahedral, dihedral and icosadeltahedral configurations fail to be global energy minima are in remarkable concordance with a theory given by Dodgson and Moore [13] originally for icosadeltahedral configurations: Using continuum elasticity theory [18] they studied the energy cost of a pair of pentamers, compared with a pure hexagonal lattice, and suggested that dislocation defects–extra fivefold coordinated points, with (necessarily) paired sevenfold coordinated points–would lower lattice strain and energy for N in the ≈ 500–1000 range. Similar reasoning should apply to the tetrahedral configurations in the $N = 78$ series and dihedral configurations in the $N = 137$ series. Our results given here are strong confirmation of Dodgson and Moores theory [13].

The fact that apparently for $N > 792$ all symmetric tetrahedral, dihedral or icosadeltahedral lattices are not global minima, along with the exponential growth in good local minima

may help explain why the number of Mo_{154} anions which self-assemble into a spherical superstructure [4] is a non–lattice number 1165, rather than, for example, 1172 the closest icosadeltahedral lattice or the tetrahedral lattice at 1218, while for small N self-assembly often produces a symmetric lattice configuration [2, 3].

For icosadeltahedral configurations for $N \leq 792$ whether or not a lattice configuration is a potential global minimum depends not only on the magnitude of N, but also apparently on the details of the lattice itself. All lattice N are listed in Tables I and II. As can be seen for $N = 42, 92, 162, 252, 362, 432, 492, 572, 642, 732$ the icosahedral lattice configuration is manifestly not the global minimum, while for the other N, the lattice configuration appears to be so.

In an icosadeltahedral lattice $N = 10(h^2 + k^2 + hk) + 2$, to go from the center of one pentamer to the center of an adjacent pentamer one moves h steps along one basis vector fo the lattice, and then k steps in the other. We noted previously [12] (also discussed in ref. [19]) that the energy in an icosadeltahedral lattice configuration with a large ratio of h to k ($h \geq k$) may be increased due to the vertices of the pentamers being closely aliged (or perfectly aligned in a lattice with $k = 0$). It has previously been noted that as N grows the icosadeltahedral lattice configuration may not be the global minimum [13, 14, 15, 16, 17], though we have not seen any explicit published accounting of the N for which the lattice fails to be a global minimum. This is given in Tables I and II (in addition to the rule that for $N > 792$ the lattice is not the global minimum). A clear pattern emerges: for an icosadeltahedral configuration with $k = 0$, besides the extremely exceptional case of $N = 12$, the icosadeltahedral lattice configuration is not the global minimum. For the three small $N = 42, 92$ and 162 the apparent global minimum configuration has exactly twelve pentamers, and no dislocation defects, but arranged in an non-icosadeltahedral configuration, likely lowering the energy cost of having the vertices of pentamers aligned. For N larger than 162 in the $k = 0$ series, the apparent global minimum incorporates dislocation defects. For $N = 432$ and higher for lattices with $k = 1$, the lattice is also not the global minimum in accordance with the notion stated above that the energy of the lattice is increased by relative alignment of the vertices of the pentamers. The data in Tables I and II may be useful in refining theoretical predictions for global enery minima: The current theory [13, 18] correctly predicts that for $N > 1000$ icosadeltahedral and tetrahedral configurations will not be global minima, but does not yet account for various cases for $N < 1000$. As well, for $k = 0$ other theoretical

work [17, 19] predicts dislocations lowering the energy for $N > 300$, but the first instance of this is found for $N = 252$.

For tetrahedral or dihedral lattices we have not yet been able to find an obvious rule or principle to predict for which N the lattice configuration is a global minimum. Indeed, while all groups using a variety of different methods find the T_h configuration a global minimum for $N = 78$ [10], and we have found similarly for $N = 306$, there are a number of $N < 100$ for which T_h configurations are not the global minima [10, 11], and also we have found that the next analogue of the global minimum for $N = 100$ which has T (though not T_h) symmetry, $N = 394$, is not a global minimum (E.L.A. and A.P.G., data not shown). And we see no obvious difference between the $N = 78$ lattice and the others to explain why not only for $N = 78$, but the next higher analogue the lattice appears to be the global minimum. Similarly, we have appreciated no obvious reason why the next D_2 analogue of 146–578–or the next D_5 analogues of 182 and 187–722 and 742–are not global minima, but the next D_5 analogue of 137–542–appears to also be a global minimum. The theory of Dodgson and Moore [13] does not predict *a priori* that defects would lower a lattice energy for an N of 306 and 542, as it does for the next analogues 1218 and 2162. Perhaps, whatever still unknown reasons that explains the good minimum for the T_h lattice for $N = 78$ and D_5 lattice for $N = 137$ also permit the $N = 306$ and 542 analogues to be global minima.

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[1] J.J. Thomson, Philosophical Magazine 7, 237-265 (1904).

[2] D. Caspar, and A. Klug, Cold Spring Harb. Symp. Quant. Biol. 27, 1 (1962).

[3] H.W. Kroto, J.R. Heath, S.C. OBrien, R.F. Curl, and R.E. Smalley, Nature 318, 162 (1985).

[4] T. Liu, E. Diemann, H. Li, A.W. Dress, and A. Muller, Nature 426, 59 (2003).

[5] S. Smale, Math. Intelligencer 20 (2), 7 (1998).

[6] E.L. Altschuler, T.J. Williams, E.R. Ratner, F. Dowla, and F. Wooten, Phys. Rev. Let. 72, 2671 (1994).

[7] T. Erber, and G.M. Hockney, G.M. Phys. Rev. Let. 74, 1482 (1995).

[8] A. Pérez–Garrido, M. Ortuño, E. Cuevas and J. Ruiz, J. Phys. A 29, 1973 (1996).

[9] J.R. Morris, D.M. Deaven and K.M. Ho, Phys. Rev. B 53, R1740 (1996).

[10] T. Erber T. and G.M. Hockney, Adv Chem Phys. 98, 495 (1997).

[11] J.R. Edmundson, Acta Cryst. A49, 648 (1993).

[12] E.L. Altschuler, T.J. Williams, E.R. Ratner, R. Tipton, R. Stong, F. Dowla and F. Wooten, Phys. Rev. Lett. 78, 2681 (1997).

[13] M.J.W. Dodgson and M.A. Moore, Rev. B 55, 3816 (1997).

[14] A. Pérez–Garrido, M.J.W. Dodgson, M.A. Moore, M. Ortuño and A. Díaz–Sánchez, Phys. Rev. Lett. 79, 1417 (1997).

[15] A. Pérez–Garrido, M.J.W. Dodgson and M.A. Moore, Phys. Rev. B 56, 3640 (1997).

[16] A. Toomre, unpublished results, discussed in [17,19]

[17] M. J. Bowick, D. R. Nelson and A. Travesset, Phys. Rev. B 62, 8738 (2000)

[18] M.J.W. Dodgson, J. Phys. A 29, 2499 (1996).

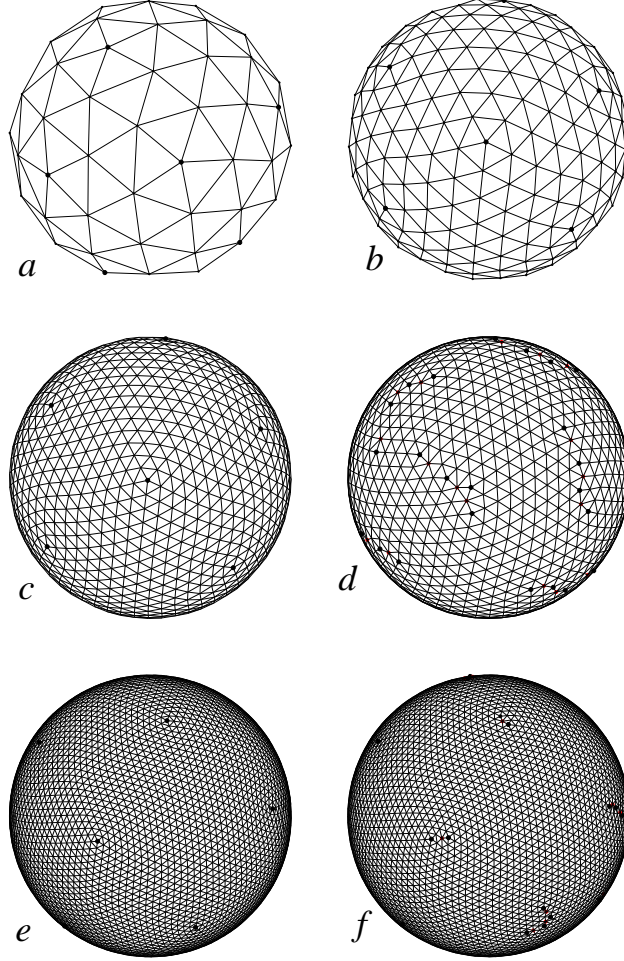[19] M. Bowick, A. Cacciuto, D.R. Nelson, and A. Travesset, Phys. Rev. Lett. 89, 185502 (2002).

FIG. 1: Tetrahedral configurations. For a) $N = 78$ ($E = 2662.04647$), b) $N = 306$ ($E = 43862.56978$), the symmetric tetrahedral lattice configuration appears to be the global energy minimum, while for $N = 1218$ c) ($E = 718284.03747$), d) ($E = 718281.63110$) and $N = 4886$ e) ($E = 11651484.51295$), f) ($E = 11651440.24177$) addition of defects to the lattice produces a configuration of lower energy. For $N = 1218$ and 4886 we give the lowest energy configuration we have found, though we cannot certain this is a global energy minima. Fivefold coordinated charges (points) (pentamers) are indicated by large black dots, and sevenfold coordinated charges (septamers) are indicated by small red dots. The rest of the charges are sixfold coordinated (hexamers). Colors in online version only.

FIG. 2: Icosadeltahedral configurations. For a) $N = 312$ ($E = 45629.36272$) the symmetric icosadeltahedral configuration appears to be a global energy minimum, while for $N = 1242$ b) ($E = 747107.43183$), c) ($E = 747106.46027$) addition of defects produces a configuration of lower energy (though not necessarily the global energy minimum). As in Figure 1 fivefold coordinated charges (points) (pentamers) are indicated by large black dots, and sevenfold coordinated charges (septamers) are indicated by small red dots. The rest of the charges are sixfold coordinated hexamers. Colors in online version only.
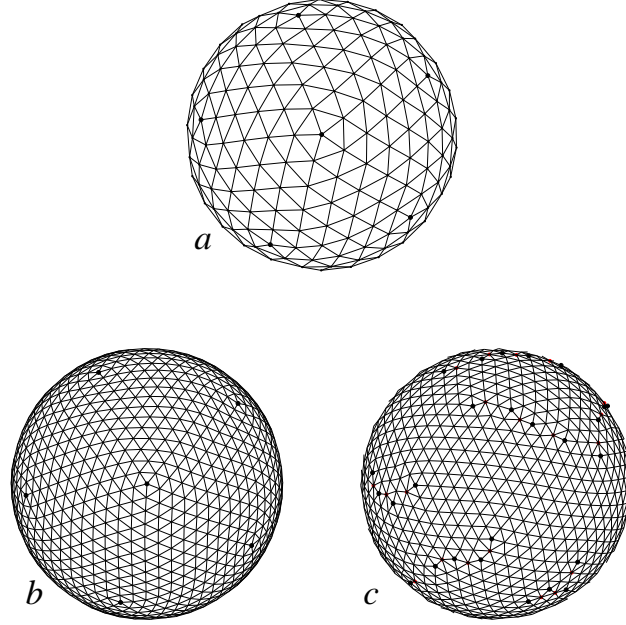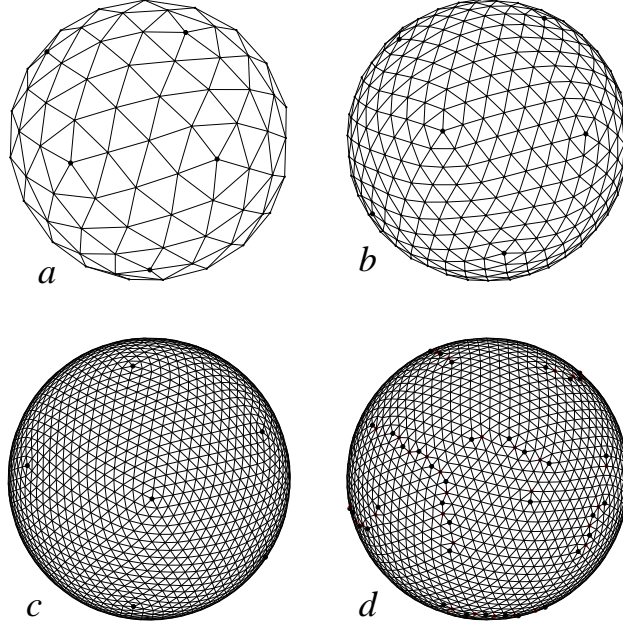
FIG. 3: Dihedral configurations. For a) $N = 137$ ($E = 8499.53449$), b) $N = 542$ ($E = 139913.69461$), the symmetric dihedral lattice configuration appears to be the global energy minimum, while for $N = 2162$ c) ($E = 2281595.05127$), d) ($E = 2281587.48735$) addition of defects to the lattice produces a configuration of lower energy. We give the lowest energy configuration we have found, though we cannot certain this is a global energy minima. Fivefold coordinated charges (points) (pentamers) are indicated by large black dots, and sevenfold coordinated charges (septamers) are indicated by small red dots. The rest of the charges are sixfold coordinated (hexamers). Colors in online version only.

TABLE I: Energy of icosadeltahedral configurations with $N < 400$. An * indicates a configuration of lower energy, though not necessarily the global minimum. For each N, here and Table II, we tried fifteen runs–random initial configurations followed by a local gradient descent–to find a configuration with an energy lower than that of the icosadeltahedral lattice. For $N = 42$, 92 and 162 the best known configuration has exactly twelve pentamers (and thus no dislocation defects), but does not have icosadeltahedral symmetry. We note that the split larger analogue of the global minimum configuration for $N = 42$ is not the global minimum configuration for $N = 162$, and neither are the split larger analogues of the $N = 92$ and 162 global minima (data not shown).

Charges		Energy
12	h= 1 k= 0	49.1652530580000
32	h= 1 k= 1	412.261274651000
42	h= 2 k= 0	732.256241038000
	*Non–icosadeltahedral	732.078107551000
72	h= 2 k= 1	2255.00119099000
92	h= 3 k= 0	3745.61873908500
	*Non–icosadeltahedral	3745.29163624500
122	h= 2 k= 2	6698.37449926100
132	h= 3 k= 1	7875.04534281600
162	h= 4 k= 0	11984.5514338730
	*Non–icosadeltahedral	11984.0503358310
192	h= 3 k= 2	16963.3383864710
212	h= 4 k= 1	20768.0530859690
252	h= 5 k= 0	29544.2821928610
	* w/defects	29543.7859569610
272	h= 3 k= 3	34515.1932926880
282	h= 4 k= 2	37147.2944184740
312	h= 5 k= 1	45629.3627238190
362	h= 6 k= 0	61720.0233978130
	* w/defects	61719.3090545160
372	h= 4 k= 3	65230.0271225660
392	h= 5 k= 2	72546.2583708950

TABLE II: Energy of icosadeltahedral configurations with $N > 400$. An * indicates a configuration of lower energy, though not necessarily the global minimum. Thus, for $N < 792$ we also cannot be certain that the symmetric icosadeltahedral configurations are the global minima.

432	h= 6 k= 1	88354.2293807250	
	* w/defects	88354.1906652260	
482	h= 4 k= 4	110318.139920155	
492	h= 7 k= 0	115006.982258289	
	*h= 5 k= 3	115005.255889700	
522	h= 6 k= 2	129655.833007858	
572	h= 7 k= 1	156037.879346228	
	* w/defects	156037.316647696	
612	h= 5 k= 4	178910.494981768	
642	h= 8 k= 0	197100.363816212	
	* w/defects	197098.637958037	
672	h= 7 k= 2	216171.432658341	
732	h= 8 k= 1	256975.527362500	
	* w/defects	256974.262894426	
752	h= 5 k= 5	271362.588212841	
762	h= 6 k= 4	278704.548700071	
792	h= 7 k= 3	301321.818305597	
812	h= 9 k= 0	316895.372099956	
	* w/defects	316892.668538128	
842	h= 8 k= 2	340988.383415978	
	* w/defects	340987.675098937	
912	h= 9 k= 1	400662.383224662	
	h= 6 k= 5	400660.132041002	
	* w/defects	400659.747279004	
932	h= 7 k= 4	418596.898209635	
	* w/defects	418595.636527970	
972	h= 8 k= 3	455654.618623736	
	* w/defects	455653.441695822	
1082	h= 6 k= 6	565703.908873765	
	* w/defects	565703.766602964	